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ACOUSTIC GRAVITY WAVE CHEMISTRY MODEL FOR THE RAYTRACE CODE

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1 March 1984

Technical Report

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This report discusses the implementation of F-region electron chemistry in the acoustic gravity wave model of the code RAYTRACE. The chemistry consists of three dominant reactions that control electron depletion in an F-region parcel that is pushed down into the higher density E-region atmosphere by the passage of a large amplitude gravity wave. The effect of electron depletion on the propagation of high frequency radio waves is shown by comparison of RAYTRACE radio propagation calculations with and without chemistry.

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ACOUSTIC GRAVITY WAVE CHEMISTRY MODEL FOR THE RAYTRACE CODE

INTRODUCTION

Nuclear explosions in the atmosphere are known to generate large amplitude internal gravity waves which propagate great distances from the explosion point and may cause modification of the ionosphere as they pass by. Such modifications may result in substantial impact on HF radio communications that use that part of the ionosphere as a reflecting point. Typical impacts on HF transmissions include: introduction of multipath, reduction in the MUF, and changes in absorption.

A detailed computer model has been generated to describe the dynamics of the acoustic gravity wave from its creation to its propagation through the ionosphere. The model is implemented in the MRC HF communications computer code RAYTRACE 1 . This note describes enhancements to this AGW model to include appropriate F-region electron density depletion chemistry.

BACKGROUND

For distances far from a nuclear explosion little is known about mechanisms causing the acoustic gravity wave. For distances closer to the explosion our understanding is better. In the model developed by McCartor, et al., in Reference 1, available data is combined with the general theoretical knowledge of the properties of the AGW to describe its dynamics. Some of the most important properties of an AGW incorporated into the RAYTRACE model and pertinent to the question of chemistry are:

- Long period, freely propagation gravity modes dominate the distant disturbances launched from low altitude sources². These modes give a fairly constant period fluctuation at a fixed range.
- 2. The long period waves tend to bend around the earth's surface. $^{\rm 3}$
- 3. The intensity of the AGW disturbances changes with altitude. It tends to grow exponentially with altitude up to about 300 km and then decreases above 300 km due to viscous dissipation.
- 4. Ionospheric plasma driven by atmospheric motion is largely confined to motion along the magnetic field lines.
- 5. The disturbances show a nearly sinusoidal variation with one or two cycles. 4
- 6. AGW's show a nearly constant period for individual stations which increased with increasing distances from the burst.
- 7. The initial motion of the ionosphere (up or down) seemed to be fixed by the magnetic field orientation.

In general, good agreement was found between the model and existing data sets on gravity waves from nuclear explosions. Not included in the implemented model however is the effect of chemistry on an electron population when it is pushed into denser atmosphere by gravity wave passage (property 4 above). F-region recombination chemistry is expected to greatly deplete the electron density for waves that have sufficient amplitude to push F-region electron parcels below about 200 km for tens of minutes.

CHEMISTRY MODEL INCORPORATION

The RAYTRACE computer program was initially developed by Jones and Stephenson at the Department of Commerce⁵ for studying HF radio communications in natural environments and was adapted to handle nuclear explosion disturbed environments by M. Frolli of Mission Research Corporation. The program traces rays through an anisotropic medium whose index of refraction varies continuously in three dimensions. The program calculates ray paths by numerically integrating Hamilton's equations. It can represent the refractive index by either the Appleton-Hartree or the Sen-Wyller formula, and has several ionospheric models for electron density (including the AGW model), perturbations to the electron density , the earth's magnetic field, and electron collision frequency.

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Since the code performs numerical integration to trace radio waves along a propagation path, it takes a number of small time steps in high gradient regions normally encountered in disturbed ionospheres to assure path correctness. Thus for each small spatial/time step the electron density and its gradient must be determined. This means that the AGW electron density model must be called for each integration point two or more times. Typical single bounce HF transmission calculations through a disturbed environment may require as many as one hundred thousand calls to the AGW model. Because of this large number of calls to the model, it was designed to run extremely fast. It did not contain any F-region chemistry which would slow the code. There are conditions however such as multiple bursts, large yields or a path close to a burst when plasma at high altitudes is pushed down to altitudes where an electron depletion can occur in one or two cycles of the AGW. Under such circumstances the incorporation of F-region chemistry is necessary to give an accurate picture of the HF propagation effects. For this reason it was felt that F-region chemistry should be available as a model option for large yield cases where chemistry may be important.

It is important however that the addition of the necessary chemistry not add significant running time to the AGW model in RAYTRACE. In fact because of the already substantial run time required to perform a RAYTRACE calculation through a modestly disturbed environment, the chemistry was chosen to be exceedingly simple and include only the dominant reactions pertinent to electron depletion. Also to avoid undo computational complexity only the nighttime chemistry (no sources) is presently implemented in the code.

CHEMISTRY MODEL

The F-region chemistry reactions have been reduced to the simple set of three reactions:

$$N_2 + 0^+ \rightarrow N0^+ + N$$
 (1a)

$$0_2 + 0^+ \rightarrow 0_2^+ + 0$$
 (1b)

$$N0^+ + e \rightarrow N + 0 \tag{2}$$

where the speed of the first two reactions is much slower than the last and determines the final electron density, N_e . A solution for the electron density at any time t given the initial density N_{e0} at t = 0 is given by

$$N_e = N_{eo} \exp(-\int \alpha dt)$$
 (3)

where α is the effective recombination coefficient given by

$$\alpha = K_1[N_2] + K_2[0_2]$$
 (4)

where

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$$k_1 = 1.3 \times 10^{-12} \tag{5}$$

and

$$k_2 = 2. \times 10^{-11}$$
 (6)

Since the electron parcel is moving up and down with the motion of the gravity wave, the $[N_2]$ and $[0_2]$ densities are functions of time.

The procedure developed to estimate densities has been to initially fit the neutral $[N_2]$ and $[0_2]$ densities with an exponential function of height h between the regions of 100 and 500 km as:

$$[N_2] = Ae^{Bh(t)}$$
 (7)

$$[0_2] = Ce^{Dh(t)} (8)$$

The recombination coefficient then becomes

$$\alpha(t) = k_1 Ae^{Bh(t)} + k_2 Ce^{Dh(t)} . \qquad (9)$$

The height, h, is the instantaneous altitude of the air parcel at time t and is given for a single burst by

$$h(t) = \Delta Z_{mx} \sin \{w(t-x/c)\} + Z_0$$
 (10)

where Z_{mx} is the maximum displacement of the parcel at distance χ from the burst: Z_0 is the initial height of the air parcel and w is $2\pi Z/\tau Bx$. For the single burst case using equations (9) and (10), the integral in equation (3) can be carried out analytically for the case where the wave has gone through two cycles. The result for that case is

$$\alpha_{mx} = \int \alpha(t)dt = 2 \exp[-K_1 A e^{BZ_0} 2\pi I_0(B \Delta Z_{mx})]$$

$$+ \exp[-K_2 C e^{DZ_0} 2\pi I_0(D \Delta Z_{mx})]$$
(11)

where I_0 is the zero order Bessel function with imaginary argument.

The result can be interpolated to a time t between zero and two cycles of the AGW by using the following approximation:

$$\int_{0}^{t} \alpha dt = \frac{\omega(t - \chi/c)}{4\pi} \alpha_{mx} + A[\cos(\omega(t - \chi/c) - 1)\cos\phi\sin\theta]$$
 (12)

where A is given by the approximate value determined by fitting equation (12) to exact calculations as

$$A = .08 \alpha_{mx}$$
 (13)

 ϕ is the magnetic azimuth and θ is the magnetic dip angle.

The single burst model for integral of $\alpha(t)$ agrees to within a few percent of the exact value determined by direct time integration of the dynamical equations. The model runs very quickly requiring only the evaluation of equations (11) and (12).

MULTIBURST MODEL CHEMISTRY

The above simple model is accurate for the single burst model since the motion of the electron parcel can be closely approximated by a single sinusoidal function that can then be integrated analytically. For the multiburst case the motion of the electron parcel is the result of a

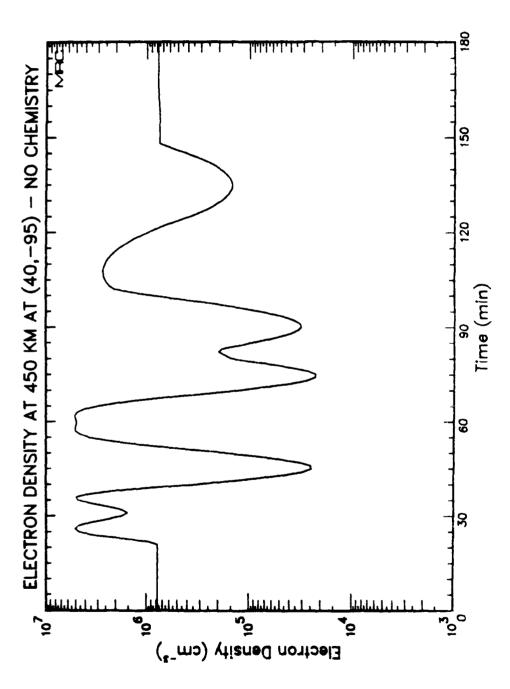


Figure 11. Same as Figure 9 but at an altitude of 450 km.

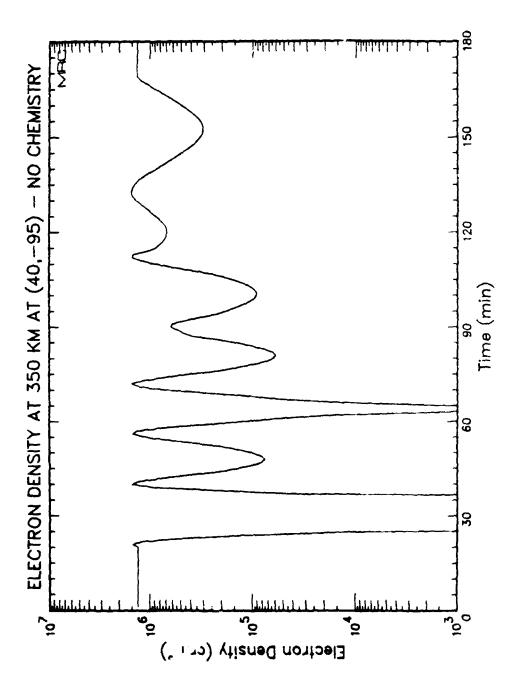
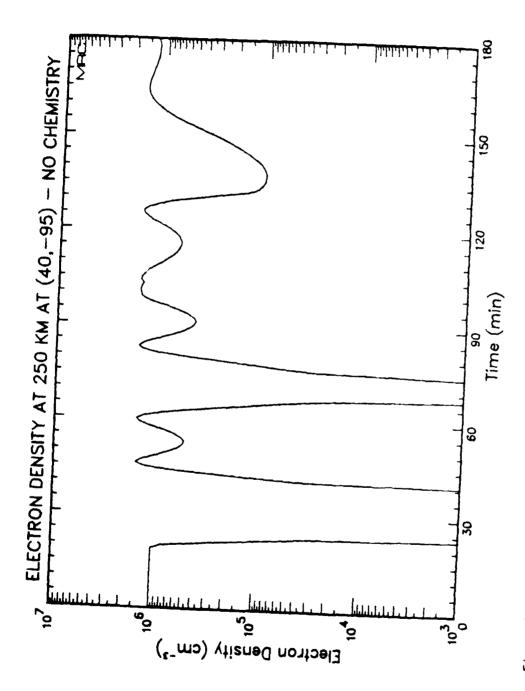
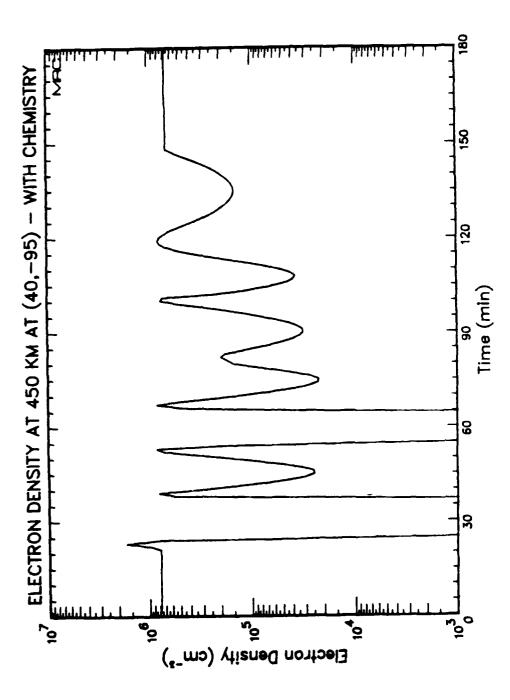


Figure 10. Same as Figure 9 but at an altitude of 350 km.



Electron density at height of 250 km as a function of time after burst time in a multiburst scenario. Same as Figure 6 except no chemistry is included. Passage of first gravity wave occurs at about 20 minutes after the first burst. Figure 9.



igure 8. Same as Figure 6 but at an altitude of 450 km.

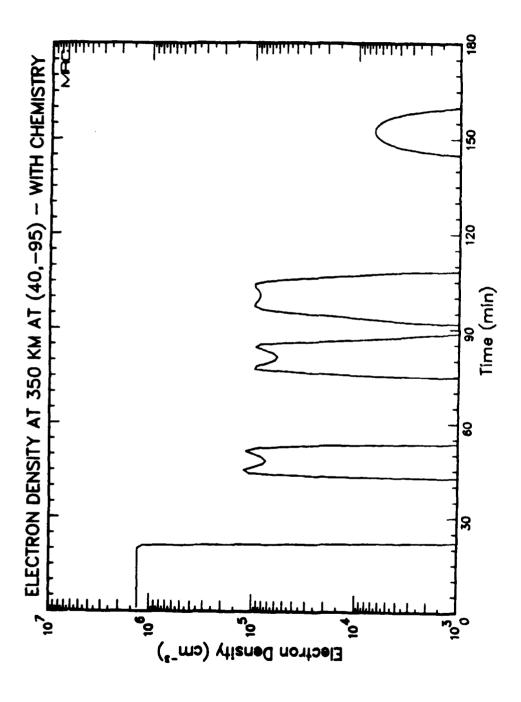
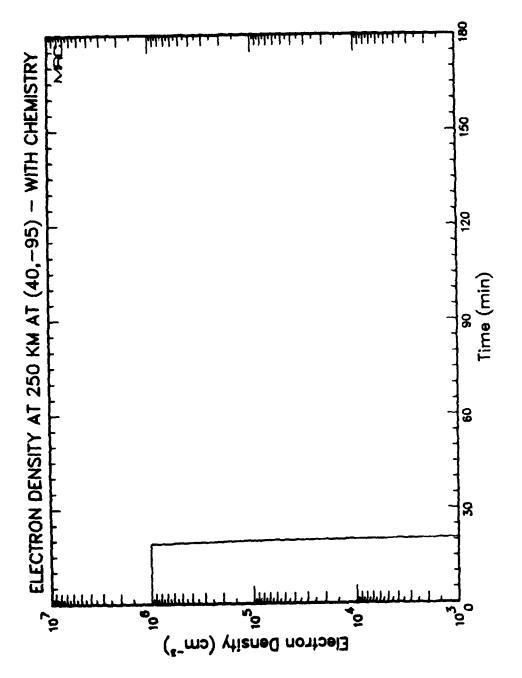


Figure 7. Same as Figure 6 but at an altitude of 350 km.



Electron density at height of 250 km as a function of time after burst time in a multiburst scenario. Chemistry is included. Passage of first gravity wave occurs at about 20 minutes after the first burst. Figure 6.

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minutes after the passage of a very large amplitude gravity wave. The wave resulted from a combination of 100 MT and 30 MT explosions detonated in a region about the zero tic on the figure. (Details of the explosion scenario have been discussed in Reference 1.)

Figure 4 shows critical frequency contours without the effect of chemistry. Figure 5 shows the same region and time but with the F region chemistry included. The chemistry model assumes a night time ionosphere with no electron production sources. It is seen in Figure 10 that large regions of electron depletion (small critical frequency) remain after the passage of the gravity wave. These regions persist for the entire night. As the wave continues to move outward from the explosion point it continues to create an expanding depletion region. This depletion region resulting from the inclusion of chemistry considerably simplifies the disturbed electron density height profile that would have been present from the passage of the gravity wave without chemistry (Figure 4). The simplified electron density height profile may reduce the absorption and multipath but may tend to increase the doppler shift in the HF signal.

Electron density time histories for the multihurst scenario used to generate Figures 4 and 5 are given in Figures 6 through 11 for slices at three heights. Figures 6, 7 and 8 show electron density time histories at 250, 350 and 450 km respectively with the chemistry turned on. Figures 9, 10, and 11 show the same slices but without chemistry. At 250 km altitude electron density is entirely depleted after the passage of the gravity wave. At higher altitudes there is less affect on the electron density resulting in an occasional depletion hole.

SINGLE BURST EXAMPLE

The effect of the passage of a gravity wave through a section of the ionosphere can be seen somewhat more clearly by looking at the

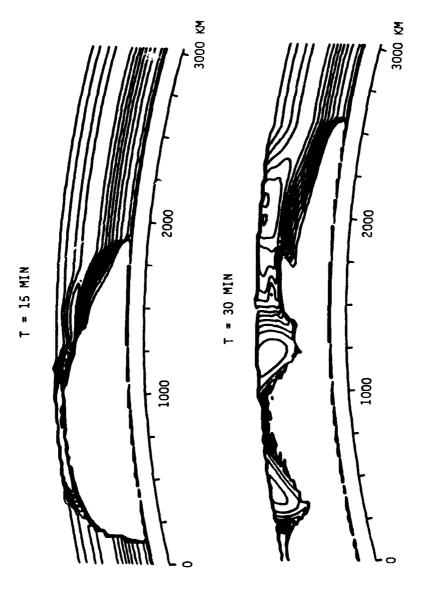
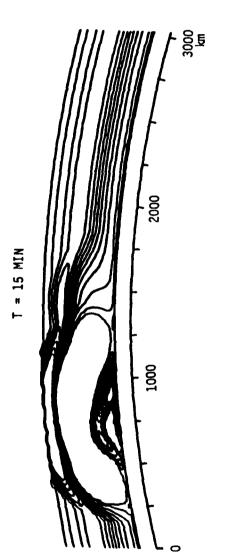
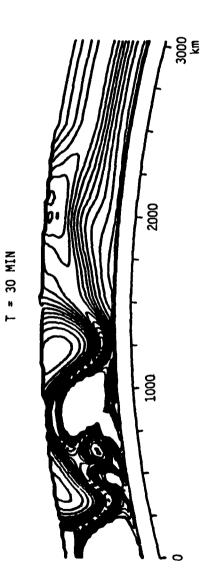


Figure 5. Critical frequency contours with chemistry.

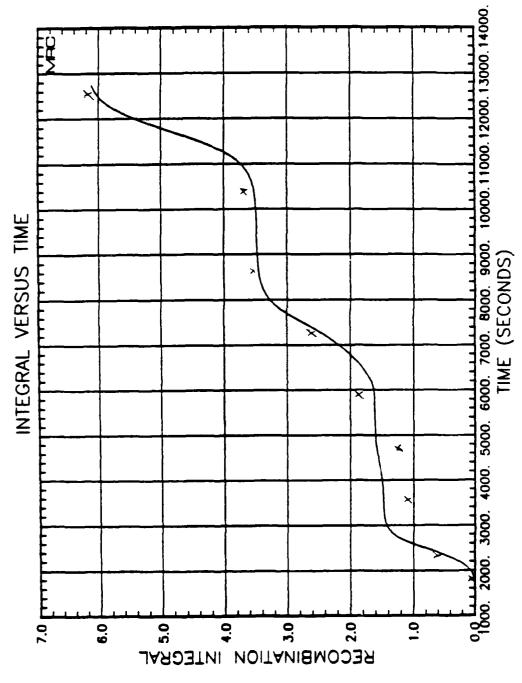
1 MHZ BETWEEN CONTOURS





1 MHZ BETWEEN CONTOURS

Figure 4. Critical frequency contours without chemistry.



Integral of recombination coefficient for multiburst case discussed in text. The solid line is true integral value, the X's are the model approximation. Figure 3.

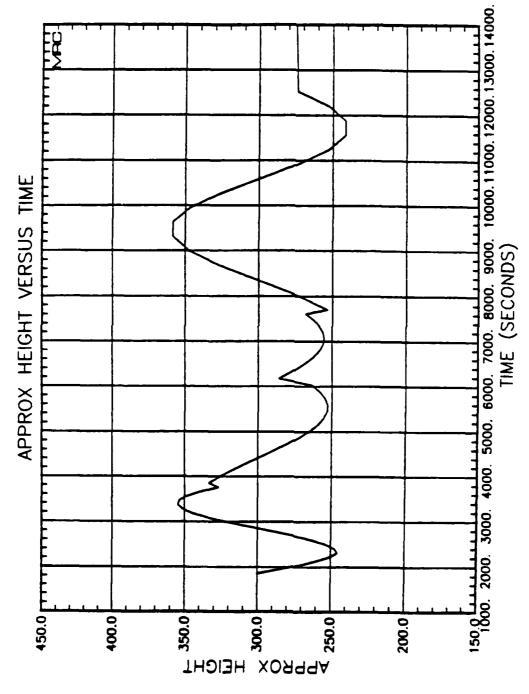
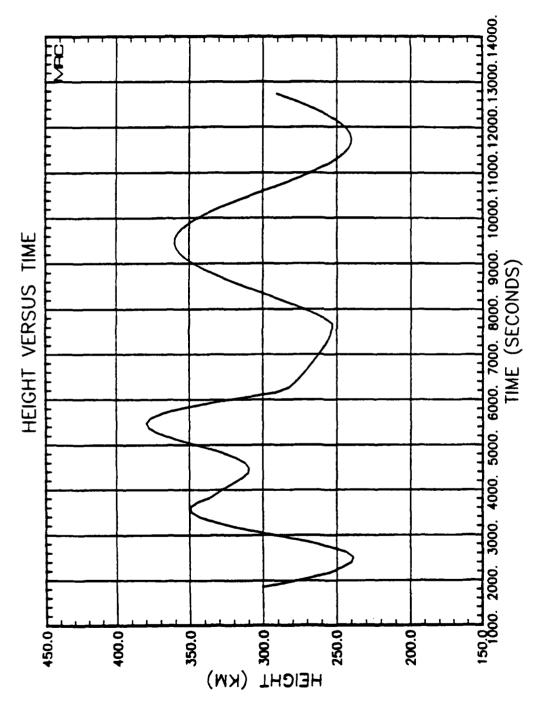


Figure 2. Model approximation to parcel dynamics given in Figure 1.



Plot of height versus time for ion parcel moving under the combined effects of three nuclear bursts. Figure 1.

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The amplitude value, $<\!\Delta Z_{m\,x}\!>$, is the frequency weighted mean amplitude of events

$$\langle \Delta Z_{mx} \rangle = \sum_{i=1}^{N_B} \frac{\Delta Z_{mxi}}{\omega_i} / \sum_{i=1}^{N_B} \left(\frac{1}{\omega_i}\right)$$
 (16)

is the minimum of the ω_i 's for the interval, and χ_{max} is the distance associated with the ω_i minimum.

An example of the motion of a parcel during multiburst scenario is given in Figure 1. Three events were interacting; they had yields of $10\,$ Mt, $1200\,$ km due north of the point of interest, $15\,$ Mt, $1500\,$ km nearly due south, and $5\,$ Mt $2000\,$ km at $60\,$ degrees azimuth.

The approximate fit to the parcel height using the multiburst model is given in Figure 2. In general the fit is quite good except for a single region near 5000 seconds where equal and nearly opposite motion drive the parcel in a way that cannot be well predicted by the simplified model.

Figure 3 shows the exact integral of a(t) (eq(12)) for the multiburst case. The approximate integral is given by the X marks for selected times. The fit of the integral is more accurate than our knowledge of either the neutral atmospheric model or the simplified chemistry model.

COMPARISON OF AGW ENVIRONMENTS WITH AND WITHOUT CHEMISTRY

Examples of the effect of F-region chemistry in the wake of a large amplitude gravity wave are seen by examining Figures 4 and 5. Figure 4 shows the critical frequency contours at 15 minutes and 30

superposition of multiple sinusoidal functions that in general will have distinct amplitudes, periods, phases and arrival times at the point of interest. Thus for multiple bursts the model becomes somewhat more complicated but can still be made to maintain most of the character of single burst chemistry model.

The primary consideration in the multiburst case is to get an accurate time history of the vertical motion of the parcel at the point of interest. This motion which is the result of the passage of the multiple AGW's past the point of interest can be expressed as the sum of sine waves i. e.,

$$h(t) - e \sum_{j=1}^{N_B} \Delta Z_{mx_j} \sin \omega_j (t - \chi_j/c) + Z_0$$
 (14)

where index, i, runs over all bursts that have

$$\frac{x_i}{c} \le t < \left(\frac{x_i}{c} + \frac{2x_i}{2}\right) \tag{15}$$

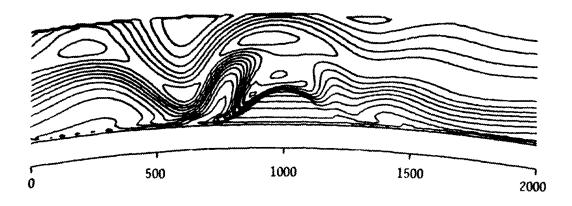
Using equation (14) in equation (9) results in an integral that cannot be evaluated exactly. A procedure was adopted where the summation is approximated over a few discrete intervals over which the integral can be done analytically. The intervals are determined by the arrival times of the gravity waves from the various bursts and the departure of the waves. Essentially a new interval is created when either a wave arrives or leaves the parcel region of interest. In a given interval the parcel position is given by

$$h(t) = \langle \Delta Z_{mx} \rangle \sin \Omega(\frac{\chi_{max}}{c}) + Z_0$$

effect of the gravity wave from a single burst. Figures 12 and 13 show contours of critical frequency without and with chemistry respectively after the passage of a gravity wave 30 minutes after a 4 Mt surface explosion. As in the multiburst case the ionosphere is greatly disturbed. The chemistry has the effect of depleting the electrons below about 250 km as seen in Figure 13.

The effect on propagation through the two environments shown in Figures 12 and 13 is illustrated in Figures 14 and 15 respectively by a fan of rays at 15 MHz propagating in a southward direction from a transmitter located at the burst point. To avoid a confusing number of lines on one plot, only the rays are plotted and not the critical frequency contours. Propagation paths can be correlated to environment by overlaying the ray paths on the appropriate Figure 12 or 13. Contrary to our initial expectations, the introduction of chemistry does not greatly improve the number of HF radio waves that propagate, although the environment is greatly simplified and many gradients are removed. The introduction of chemistry does improve somewhat the distance of waves that do propagate merely because it moves the reflection layer higher.

The effect of the chemistry is further illustrated by electron density height profiles shown in Figures 16 and 17 for the single burst scenario. The profiles shown are considered nighttime profiles that have densities normally seen in daytime. They are taken at a point 1000 km south of the burst point at times labeled on the figures. Each profile at succeeding times is offset by 10 from the previous time to accommodate objecting many times on a single frame. The profiles that result from the passage of the gravity wave when no chemistry is running are fairly smooth with height. Profiles that result when chemistry is running have large reductions in density between 100 km (the bottom of the model) and about 250 km. The straight vertical line in the profiles taken with chemistry indicate that the electron density is pegged at 1000 cm**-3.



1 1 11

Figure 12. Contours of critical frequency from passage of a gravity wave from a single 4 Mt explosion. No chemistry calculations are performed.

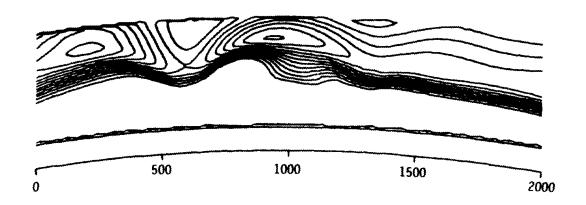


Figure 13. Same as Figure 12 except with chemistry turned on.

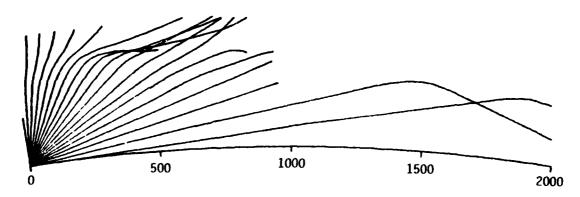


Figure 14. A fan of HF propagation rays at 15 MHz transmitted from ground zero through the electron environment described in Figure 12.

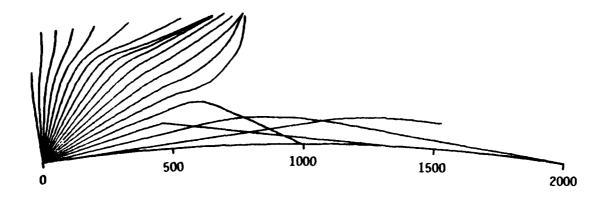
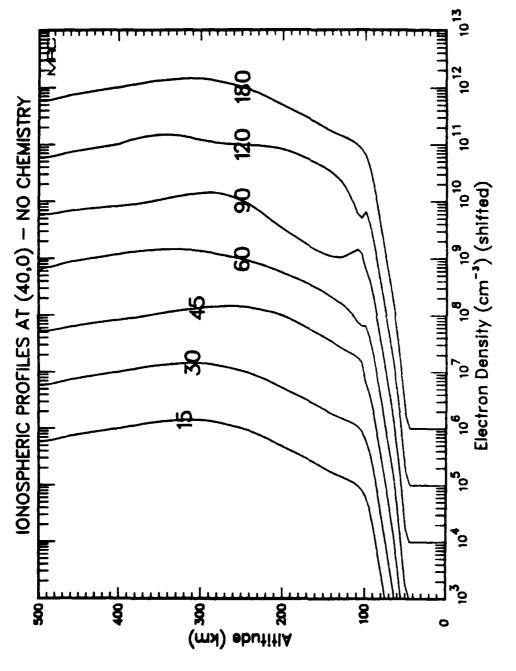


Figure 15. Same as Figure 14 except that rays are propagating through the environment in Figure 13.



Electron density height profiles taken at 1000 km from the burst point through the 30 minute environment with no chemistry. Figure 16.

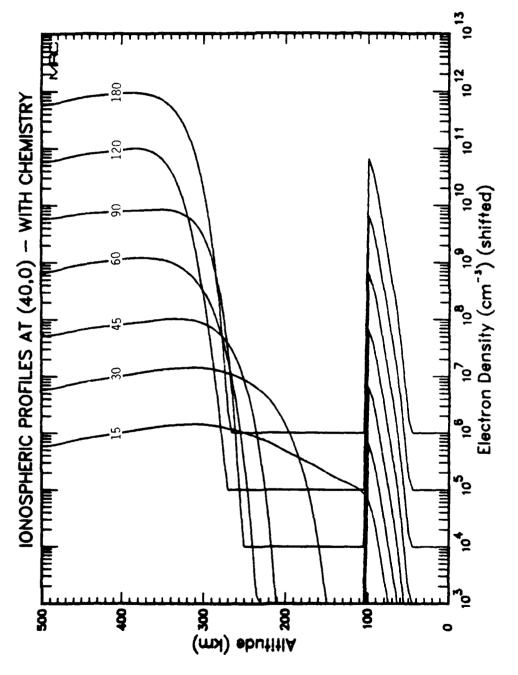


Figure 17. Same as Figure 16 except the environment had density turned on.

CHEMISTRY MODEL DEFICIENCIES

A major drawback of the model as it is now implemented is that the chemistry model is very simple and the ionosphere is not always stable to application of the model. This defect can be overcome by putting an ionosphere into the code and running it for a sufficiently long simulation time to bring the ionosphere to equilibrium and then using this ionosphere as the one through which the gravity wave propagates. This method has the defect that the exact ionospheric conditions desired may not be simulated. A more correct procedure would be to modify the chemistry such that the user-specified ionosphere is left stable. This procedure is considerably more difficult than modifying the ionosphere to fit the simple chemistry and it may also add considerable run time to a RAYTRACE calculation.

IMPLEMENTATION OF AGN CHEMISTRY INTO RAYTRACE CODE

The RAYTRACE code is organized in a modular fashion so that calculations can be performed using input-selected environment models for electron density and electron density perturbations.

There is only one input flag that needs to be set to turn on the AGW chemistry model and that is word 103 in the "W" array which is loaded on input (see the RAYTRACE documentation, reference 6). The internal flag name is CHMFLG. AGW chemistry is turned on when W103 (CHMFLG) is set to 1. No other parameters or data are required to run the AGW chemistry.

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